Invited Article
Development of CFD Simulations in Support of Air Quality Studies

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Overview

Computational Fluid Dynamics (CFD) simulations of pollutant concentrations within roadway and building microenvironments is feasible using high performance computing CFD models are emerging as a promising technology for such assessments, in part due to the advancing power of computational hardware and software. The results of CFD simulations can both be directly used to better understand specific case studies as well as be used to support the development of better-simplified algorithms that may be generally applied to complex situations. However, the tools are not well evaluated for air quality modeling and best-practice methodologies have not been established. A program has been ongoing over the past few years at the US EPA in collaboration with Fluent, Inc scientists to develop applications using the Fluent CFD software and work toward establishing best practices. Unlike most currently used regulatory air quality models, CFD simulations are able to treat for topographical details such as terrain variations and building structures in urban areas as well as local aerodynamics and turbulence. CFD simulations have the potential to yield more accurate solutions than existing regulatory air quality models because CFD models solve the fundamental physics equations including the effects of detailed three-dimensional geometry and local environmental conditions. Development and application of CFD simulations are being advanced through case studies for simulating air pollutant concentrations from sources within open fields and within complex urban building environments. CFD developments are being evaluated by comparing with both wind tunnel model and field measurements. Additional information about these ongoing developments is covered by Huber et al. (2005) and Tang et al. (2005).

Prior to September 11, 2001 developments of CFD were begun to support air quality applications assessing the impact from usual sources of pollution. There is a need to properly develop the application of CFD methods in support of air quality studies involving pollution sources near buildings at industrial sites and roadways. While this original work continues, following September 11, 2001 there was a need to model the transport of potential emissions from "ground zero" at the New York World Trade Center (WTC) area. Much has been learned and developed over the past few years through research and development.

Originally the plans were to develop CFD applications under a more modest progression of urban complexity. Rising to the need to study lower Manhattan, which is one of the most complex urban building environments on earth, presented great challenges. By learning to overcome many of these challenges, future more common modeling of air quality in urban building environments should be easier. Plume dispersion in the absence of buildings is generally simulated with standard plume dispersion models for point and line source pollutant emissions. The development of CFD methods and applications in urban building environments is critical when it is important to accurately estimate potential human exposures to local sources of a toxic contaminant. In the absence of being able to measure everything we need to know in the field, finely resolved numerical models are necessary to fully understand relationships between local pollutant sources and air concentrations along their pathways to exposure. CFD simulations have great potential for supporting both urban air quality and homeland security studies.

Software

FLUENT, which is a general purpose computational fluid dynamics code that solves the governing equations for the conservation of mass, momentum, energy, and scalars such as a pollutant, is being used. The codes multiphase models, moving domain models, and turbulence models are being applied. Developing quality mesh for the complex array of buildings found in lower Manhattan has been particularly challenging. The process is much smoother for idealized building shapes where the model may be developed directly though the GAMBIT code. Computational Engineering International (CEI) mesh and Visualization software is also being used. Setting up a CFD model of an urban area requires a building database. Buildings for the New York City studies were developed from a database licensed with Vexcel Corporation.

Atmospheric Boundary Layer

For atmospheric flows the segregated solver using implicit discretization is being used. In general, second order calculations are being used. Initial developments are working with the steady-state solutions for the Reynolds-Averaged Navier-Stokes (RANS) governing equations for momentum. The realizable k-ε turbulence modeling option is presently the default. There are several other k-ε options that are being evaluated for future application. In the future higher order turbulence closure models including Reynolds Stress Models (RSM) and Large Eddy Simulation (LES) within the framework of unsteady

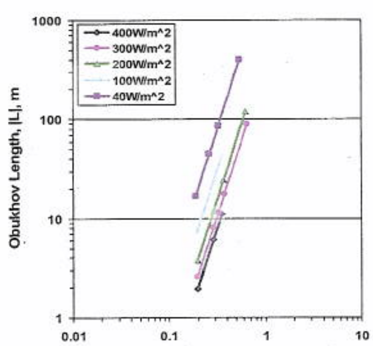

Figure 1. Monin-Obukhov theory applied to a range of case studies

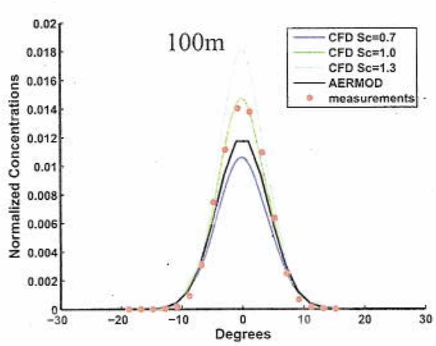

Figure 2. Example Project Prairie Grass case.

solutions will be evaluated.

Simulation of the atmospheric boundary layer is critical to modeling plume dispersion. Boundary layer turbulence can be simulated as characterized by surface roughness (characterized by z_0 and surface stress u_*) and surface heat flux (characterized by the Obukhov length L). The "law of the wall" is applied to develop an atmospheric boundary layer oncoming as boundary conditions to the study zone with buildings. No work has yet been started to evaluate strongly stable stratified flow. Figure 1 presents a summary of simulated Obukhov length (L, m) versus surface friction velocity that result from a range of simulations. These results are found to compare well with Monin-Obukhov theory. Figure 2 presents example comparisons of the crosswind profiles of normalized concentrations compared with field measurements from project Prairie Grass (Barad, 1958), demonstrating comparability with the measurements and the AERMOD regulatory plume model (Cimorelli et al., 2005). Three turbulent Schmidt Numbers are being evaluated.

Simulations from WTC Studies

CFD applications have been under development to reconstruct the dust/smoke plume following the events at the New York City World Trade Center on September 11, 2001. The scope of the reconstruction has 3 stages:

a) the plume following airplane impact but prior to the collapse of the towers
b) during and immediately following the tower collapse
c) the days following September 11 when emissions from "ground zero" could be significant.

Parts b) and c) are the key developments and briefly presented in this summary. A large amount of momentum and kinetic energy is generated by the collapsing tower. During the collapse potential energy is being converted to kinetic energy. The flow impingement created by a collapsing tower creates vortex structures which transport gaseous constituents and particulate matter radially outward from the base of the towers. These materials were dispersed though lower Manhattan into the surrounding Metropolitan area. Nearby the collapsed towers the material was transported radially in all directions. However, this radial impulse created by the collapsed tower is short lived and soon the material is caught by the prevailing winds. Figure 3 presents an example near surface (H= 5 m above ground) wind field. Immediately following the completion of the collapse (T= 15 s) an impulse radiating out from the tower base is shown. Maximum velocities of 30-40 m/s range were short lived. Figure 4 presents an example of the smoke and

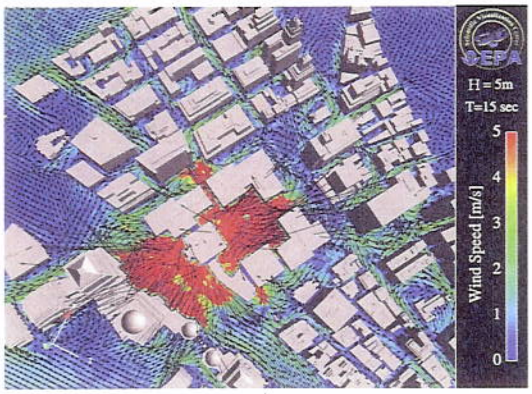

Figure 3. Surface winds immediately following the building collapse.

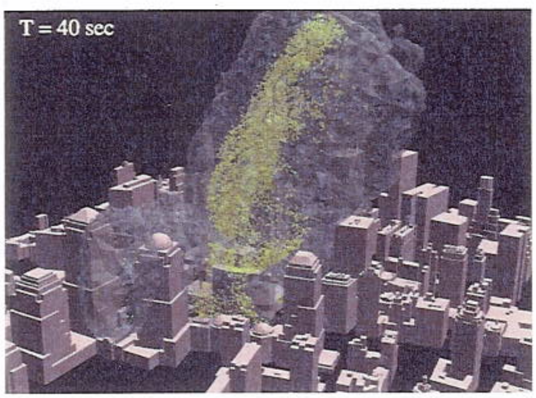

Figure 4. Example visualization of outer boundary of smoke and of a particle cloud immediately following the building collapse.

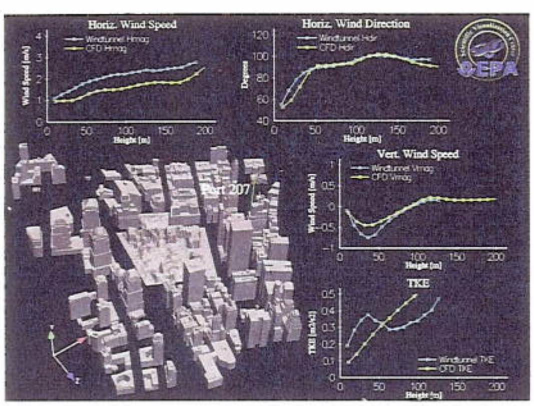

Figure 5. Example comparisons between CFD model and wind tunnel model vertical profiles of horizontal wind. speed and direction, vertical wind speed, and TKE for Westerly winds case. (Wind tunnel measurements provided by Dr Steven Perry, US EPA)

small particle plume following the collapse of the North Tower. The suspended particles are concentrated in the central core of the plume since they disperse less rapidly relative to the smoke as outlined by the grey shading. Figure 5 presents a comparison of horizontal wind speed, horizontal wind direction, vertical wind speed, and TKE for a vertical profile at Port 207 located as the green pole in the figure. Note that degree on the wind direction scale represents direction toward which the wind vector points (West winds are reported as 90 degrees). This is for a Westerly winds case. The horizontal wind speed and direction match well. There are some zones with strong wind shear and which are well matched. A comparison with all the wind tunnel model measurements is being made. Additional information of the numerical and wind tunnel modeling support for the WTC studies can be found in Huber et al. (2004) and Perry et al. (2004).

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